APPENDIX II

201-15232B

ROBUST SUMMARIES OF STUDIES USED TO CHARACTERIZE THE CRUDE BUTADIENE C4 CATEGORY

PHYSICO-CHEMICAL ROBUST SUMMARIES

Melting Point

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Chemical / Calculated MP (°C) / Measured* MP (°C) Isobutane: -132.55 / -138.3 n-butane: -120.28 / -138.2 isobutylene: -130.88 / -140.4 cis-butene-2: -120.41 / -105.5 trans-butene-2: -120.41 / -105.5 butene-1: -121.74 / -145.0 1,3-butadiene: -123.21 / -108.9 * Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured

	values which are taken from SRC's PHYSPROP Database. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the melting range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated values, products in this category can have a melting range of -132.55 to -120.28 °C. Based on the measured values, products in this category can have a melting range of -145.0 to -105.5°C.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include calculated values based on the chemical structure and experimental values available in the

	MPBPWIN program and represent a potential melting range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Boiling Point

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point estimations performed by MPBPWIN are based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. **34**: 581-587.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	<u>Chemical</u> — <u>Calculated BP (°C)</u> — <u>Measured* BP (°C)</u> Isobutane — 3.21 — -11.7 n-butane — 19.58 — -0.5 isobutylene — 10.18 — -6.9 cis-butene-2 — 27.82 — 0.8 trans-butene-2 — 27.82 — 0.8 butene-1 — 17.57 — -1.3 1,3-butadiene — 15.55 — -4.4 * Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated <u>Crude Butadiene C4.</u> The seven chemicals selected to represent the boiling range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene category

	products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated values, products in this category can have a boiling range of 3.21 to 27.82 °C. Based on the measured values, products in this category can have a boiling range of -11.7 to 0.8°C.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential boiling point range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "boiling point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Vapor Pressure

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure estimations performed by MPBPWIN are based on the average result of the calculation methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Chemical — Calculated VP (hPa) — Measured* VP (hPa) Isobutane — 3.45 E^3 — 3.08 E^3 n-butane — 2.41 E^3 — 2.43 E^3 isobutylene — 2.97 E^3 — 3.08 E^3 cis-butene-2 — 2.31 E^3 — 2.33 E^3 trans-butene-2 — 2.31 E^3 — 2.33 E^3 butene-1 — 2.48 E^3 — 3.00 E^3 1,3-butadiene — 2.73 E^3 — 2.81 E^3 * Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is

	why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the vapor pressure range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated values, products in this category can have a vapor pressure range of 2.31 E^3 to 3.45 E^3 hPa. Based on the measured values, products in this category can have a vapor pressure range of 2. 33 E^3 to 3.08 E^3 hPa.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential vapor pressure range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. MPBPWIN is contained in the computer program EPIWIN. 1999. Estimation Program

	Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "vapor pressure". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Partition Coefficient

Test Substance*:	Other TS
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. **84**:83-92.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Chemical / Calculated log K_{ow} / Measured* log K_{ow} Isobutane 2.23 2.76 n-butane 2.31 2.89 isobutylene 2.23 2.34 cis-butene-2 2.09 2.31 trans-butene-2 2.09 2.33 butene-1 2.17 2.40 1,3-butadiene 2.03 1.99 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the partition coefficient range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene

	category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated K_{ow} values, products in this category can have a partition coefficient range of 2.03 to 2.31. Based on the measured K_{ow} values, products in this category can have a partition coefficient range of 1.99 to 2.89.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include calculated values based on the chemical structure and experimental values available in the KOWWIN program and represent a potential partition coefficient range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "partition coefficient". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Water Solubility

Test Substance*:	Other TS
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. **15**:100-106. 1995.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Chemical / Calculated WS (mg/L) / Measured* WS (mg/L) Isobutane 496.4 175.1 n-butane 424.1 135.6 isobutylene 495.6 399.2 cis-butene-2 652.7 423.5 trans-butene-2 652.7 407.1 butene-1 557.7 354.8 1,3-butadiene 732.4 792.3 * Experimental K_{ow} values supplied by the WSKOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the water solubility range of this category are C4 hydrocarbons that are common across the 10 CAS numbers. Crude butadiene

	category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated K_{ow} values, products in this category can have a water solubility range of 424.1 to 732.4 mg/L. Based on the measured K_{ow} values, products in this category can have a water solubility range of 135.6 to 792.3 mg/L.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include values estimated using calculated K_{ow} and experimental K_{ow} values available in the WSKOWWIN program and represent a potential water solubility range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "water solubility". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

ENVIRONMENTAL FATE ROBUST SUMMARIES

Photodegradation (Direct)

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source: **Light Spectrum:** • **Wave length value (upper/lower)**	Not applicable Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, photolysis will not significantly contribute to the degradation of chemicals in the Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). The Crude Butadiene C4 Category includes two process streams: • **C4 Crude Butadiene** • **Butadiene Unit Heavy Ends** Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, products in this

	category do not contain component chemicals that will undergo direct photolysis. **The Crude Butadiene C4 Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons. Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the two process streams in this category are: • **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. • **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

	Photolysis of Hydrocarbons The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g., infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule. The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule. A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2):

<table>
<tr><td></td><td>
<table>
<tr><td rowspan="2">Hydrocarbon</td><td colspan="2">l below 290 nm</td></tr>
<tr><td>l_{max}</td><td>e</td></tr>
<tr><td>Ethylene</td><td>193</td><td>10,000</td></tr>
<tr><td>1,3-Butadiene</td><td>217</td><td>2,090</td></tr>
</table>
</td></tr>
<tr><td>Direct Photolysis**: (cont.)

Results: half-life, % degradation, quantum yield</td><td>Olefins with one double bond, two conjugated double bonds, or multiple un-conjugated bonds, which constitute the majority of the chemicals in the Crude Butadiene C4 Category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).

Products in the Crude Butadiene C4 Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

References
1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA.
2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.
3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.</td></tr>
<tr><td>Indirect Photolysis**:

• Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life</td><td>Not applicable</td></tr>
<tr><td>Degradation Products**:

• Note: Identification, concentration</td><td>Unknown</td></tr>
</table>

Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Not applicable
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

** In IUCLID, provide addtional discussion if needed in the results freetext

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Photodegradation (Indirect)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: $1.5\ E^{6}$ OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable
Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (1,2). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (3). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon

average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
Isobutane	52.6	$2.4 E^{-12}$
n-butane	48.8	$2.6 E^{-12}$
isobutylene	2.5	$51.7 E^{-12}$
cis-butene-2	2.3	$56.7 E^{-12}$
trans-butene-2	2.0	$64.3 E^{-12}$
butene-1	4.7	$27.4 E^{-12}$
1,3-butadiene	1.9	$66.6 E^{-12}$

* Atmospheric half-life values are based on a 12-hr day.

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the atmospheric half-life range of this category are C4 hydrocarbons that are common across the 10 CAS numbers listed under Test Substance. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (4).

References:

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442.
2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.
3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.
4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4

	Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products:** • **Note: Identification, concentration**	Unknown
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Atmospheric oxidation vial hydroxyl radical can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 1.9 to 52.6 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability: (FT - RL)	(2) Reliable with restrictions The results include values calculated using the AOPWIN program and represent a potential atmospheric half-life range for products with the 10 CAS numbers listed under Test Substance.
Reference: (FT - RE)	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".
** In IUCLID, provide additional discussion if needed in the results freetext
FT - Freetext
IUCLID fields include:
RL - Reliability
TC - Test Conditions

RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Hydrolysis (Stability in Water)

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type): **GLP (Y/N):**	Not applicable Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: (FT - RS) **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	**Summary** In the environment, hydrolysis will not contribute to the

degradation of chemicals in the Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes two process streams:

- **C4 Crude Butadiene**
- **Butadiene Unit Heavy Ends**

Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.

The Crude Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the two process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are

predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Crude Butadiene C4 Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3).

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4). The chemicals in this category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Crude Butadiene C4 Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High

	Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "hydrolysis". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Transport / Distribution (Fugacity)

Test Substance*:	Other TS
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guide line):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physical properties input into the model are those calculated by the EPIWIN Estimation v 3.04 program (1) or supplied by the databases of experimental values contained with EPIWIN. Output data from the equilibrium model provides basic information on the potential distribution of chemicals between selected environmental compartments (i.e. air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of partitioning data for compone nt chemicals is an estimate of the partitioning behavior for category products. Calculated* Measured** Percent Distribution Percent Distribution Chemical Air Water Air Water Isobutane 99.99 0.01 99.99 0.01 n-butane 99.98 0.02 99.99 0.01 isobutylene 99.98 0.02 99.99 0.01 cis-butene-2 99.97 0.03 99.98 0.02 trans-butene-2 99.97 0.03 99.98 0.02

	butene-1 99.98 0.02 99.99 0.01 1,3-butadiene 99.97 0.03 99.97 0.03 * Distribution values determined using input data calculated by the EPIWIN program **Distribution values determined using input data supplied by the EPIWIN program experimental databases (EXPKOW.DB, EXP_MBVP.DB, and EXP_MBVP.DB) which contain more than 11,000 organic compounds with reliably measured values. Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as less than 0.01%. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the transport / distribution range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see Test Substance) and can represent a significant proportion of a product. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-

	Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Products in the Crude Butadiene C4 Category are expected to distribute to air with a small percentage partitioning to water.
Reliability: (FT - RL)	(2) Reliable with restrictions The input data used to run the EQC Level I model include estimated values calculated by the EPIWIN program based on chemical structure, and experimental values supplied by the EPIWIN program databases. The partitioning data represent a potential distribution range for products with the 10 CAS numbers listed under Test Substance. Computer modeling is an accepted method of assessing environmental distribution of chemicals.
Reference: (FT - RE)	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "transport / distribution". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Biodegradation

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type): **GLP:**	Not applicable Not applicable
Year (study performed):	Not applicable
Inoculum:	Not applicable
Exposure Period:	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, replication, test conditions.**	Not applicable
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Not applicable
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	**SUMMARY** In the environment, biodegradation will not contribute significantly to the loss of chemicals in products from the

Crude Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes two process streams:

- **C4 Crude Butadiene**
- **Butadiene Unit Heavy Ends**

Ten CAS numbers (see Test Substance) identify products derived from these process streams. The products contain various chemicals composed of carbon and hydrogen. As discussed below, products in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that products from this category will partition to environmental compartments where they could be degraded by bacteria.

The Crude Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." The CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the three process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process.

C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

Biodegradation of Hydrocarbons

Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.

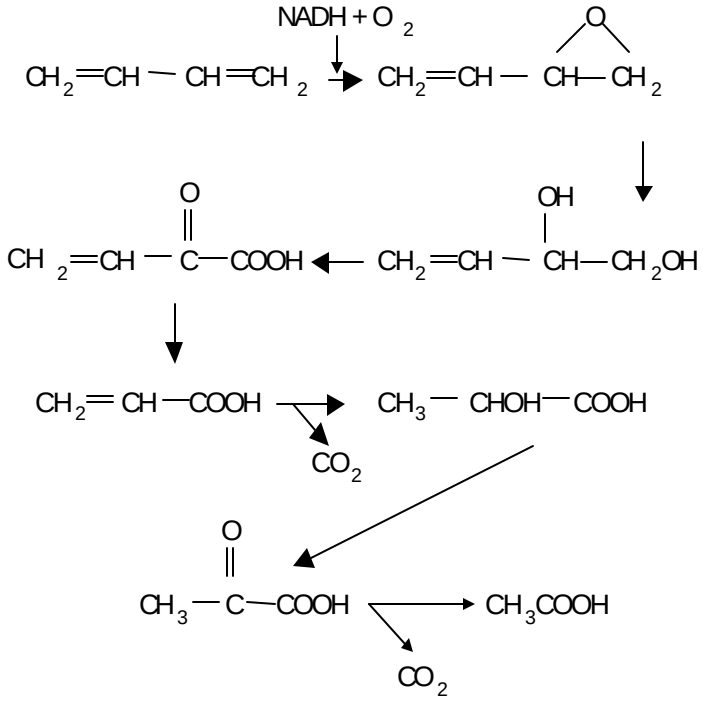
Products in the Crude Butadiene C4 Category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C5. However, the *Full-Range Butadiene Concentrates* process stream from this category, can contain hydrocarbons greater than C4. These chemicals when isolated individually are not gaseous, but relatively volatile liquids under most environmental conditions.

Several hydrocarbons as well as products that are mixtures of hydrocarbons with carbon numbers greater than C4 have been shown to biodegrade. If released to the environment, biodegradation of these chemicals will occur primarily in aquatic and terrestrial habitats. There is sufficient biodegradation data on hydrocarbons in this category that are greater than C4 to show that these chemicals have a potential to biodegrade to a great extent and not persist in the environment (see the *C5 Noncyclics, Low Benzene Naphtha, and High Benzene Naphtha* HPV Chemical Program test plans from the Olefins Panel of the American Chemistry Council, for specific data and a more detailed discussion of the biodegradability of selected hydrocarbons greater than C4.) The larger proportion of chemicals from this category are gaseous. Consequently, their availability to microbial degraders will be significantly limited.

Component chemicals from all three process streams in this category are simple hydrocarbons, the majority of which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical

attack) for specific degradation rates of selected chemicals from this category; AOP data were developed for this category under the HPV Chemical Program]. All chemicals from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment.

Products from the Crude Butadiene C4 Category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for one of the major chemicals, 1,3-butadiene, in this category that demonstrates that it can be biodegraded. Experimental studies to determine a catabolic pathway for 1,3-butadiene as mediated by a *Nocardia* sp. (3) resulted in the following proposed series of reactions:



The intermediary metabolic steps depicted above result in the production of acetic acid, CH3COOH, which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (2).

The potential biodegradability of some of the higher molecular weight components including benzene, toluene, xylene, ethylbenzene, and naphthalene has been summarized and metabolic pathways leading to their biodegradation have

	been described (4). These compounds have been shown to biodegrade to high extents such that if they were to partition to either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment. In summary, because the C4 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Chemical components of this category that are greater than C4 also have a potential to partition to the air to a great extent, where they will also degrade rapidly in a similar manner. However, they also have a potential to partition to aquatic and terrestrial environments where they are subject to biological processes that can result in their rapid biodegradation. Overall, products from this category and their component chemicals are expected to degrade rapidly in the environment and not persist. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA. 3. Watkinson, R.J. and H.J. Somerville. 1976. The Microbial Utilization of Butadiene. Shell Research Limited, Sittingbourne Research Centre, Kent, UK. 4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA.
Reliability: (FT - RL)	Not applicable
Reference: (FT - RE)	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "biodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

HUMAN HEALTH ROBUST SUMMARIES

Acute Toxicity

Test Substance	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
Method	
Method/guideline followed	OECD 402.
Type (test type)	Acute inhalation.
GLP	Yes.
Year	1982.
Species/Strain	Rat/Fischer 344.
Sex	Males and females.
No. of animals per sex per dose	5/sex.
Vehicle	Not applicable.
Route of administration	Inhalation (gas).
Test Conditions	A group of ten rats (age: 12 weeks, weight: 143-234 grams) were exposed to 5,300 mg/m3 (2,331 ppm) of the test substance in air for four hours. Analytical chamber concentrations were determined by gas chromatography every 15 minutes during the exposure; a single particle size sample was taken to show the absence of aerosol. Body weights were recorded prior to exposure and 7 and 14 days post-exposure. Individual clinical observations were recorded pre-exposure and daily for 14 days post-exposure. The rats were sacrificed on the fourteenth day and a gross necropsy performed.
Results	
LC50	Rat LC50 (4 hour) = >5,300 mg/m3 (2,331 ppm)
Remarks	Observations noted following exposure were two male rats with respiratory sounds/wheezing or hyperexcitability and one female with minimal porphyrin around the eyes. All rats were normal from Days 2-14. No significant necropsy findings were reported, except one female with an ovary filled with red fluid. Body weight gains appeared normal.
Conclusions	
(study author)	No mortality or significant adverse effects were observed in rats exposed to 5,300 mg/m3 (2,331 ppm) of the test substance.
Data Quality	
Reliability	Reliable without restrictions. Guideline study.
References	Gulf Oil Chemicals Company (1982). Acute LC50 Inhalation Toxicity Test in Rats with Butadiene Feedstock. Unpublished report (Project #82-060).

Other	Robust Summary prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	19-Oct-99

Acute Toxicity

Test Substance	1,3-butadiene CAS# 106-99-0
Method	
Method/guideline followed	Other.
Type (test type)	Acute inhalation.
GLP	Pre-GLP.
Year	1969.
Species/Strain	Rat and mouse (strains not specified).
Sex	Not specified.
No. of animals per sex per dose	Not specified.
Vehicle	Not applicable.
Route of administration	Inhalation (gas).
Test Conditions	Age, number, and sex of test animals not specified. Number of groups and exposure concentrations not specified. Dynamic flow exposure system; no description of exposure chambers or conditions. Rats exposed four hours; mice exposed two hours. No post-exposure observation period - mortality study only. Exposure concentrations "controlled" by gas chromatography.
Results	
LC50 with confidence limits	Rat LC50 (4 hour) = 285 mg/L (219-370 mg/L $p \leq 0.05$) Mouse LC50 (2 hour) = 270 mg/L (251-290 mg/L $p \leq 0.05$)
Remarks	No clinical observations or necropsy findings reported. Objective of study was to determine hydrocarbon concentrations in various tissues at lethal exposure concentrations.
Conclusions	
(study author)	LC50 value reported to be 285 mg/L (129,000 ppm) in rats, 270 mg/L (122,000 ppm) in mice.
Data Quality	
Reliability	Not assignable. Lethality study only; insufficient experimental detail to assess quality.
References	Shugaev, B.B. (1969) Concentrations of Hydrocarbons in Tissues as a Measure of Toxicity. Arch. Environ. Health 18:878-882.
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	13-Oct-99

Acute Toxicity

Test Substance	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene
Method	
Method/guideline followed	Other.
Type (test type)	Irritation screen in rabbits.
GLP	Yes.
Year	1985.
Species/Strain Sex	Rabbit (New Zealand White). 1 male, 1 female.
Vehicle	Not applicable.
Route of administration	Eye and skin.
Remarks For Test Conditions	Two young adult rabbits were evaluated for eye and skin irritation. The test substance was dispensed immediately prior to dosing into a flask packed in dry ice. On the first treatment day, 0.1mL of the test substance was instilled into one eye of each rabbit. Irritation was scored at 24, 48, and 72 hours. The untreated eye served as the control. Twenty-four hours after treatment of the eye, 0.1mL of the test substance was applied to the skin of the rabbits and occluded with a rubber dam. The test sites were evaluated 1, 3, and 7 days after dosing.
Results	
Remarks	The eye irritation scores were 0 at all observation intervals. The treated skin sites were virtually free of irritation at all observation intervals.
Conclusions	
(study author)	The test substance is estimated not to be irritating to the eye or skin.
Data Quality	
Reliability	Reliable with restrictions. Screening study.
References	Mobil Environmental and Health Sciences Laboratory (1985). Irritation Screen of Butadiene Concentrate in Albino Rabbits, Unpublished report (Study No. 41652).
Other	Robust Summary prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	24-Oct-99

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	1,3-butadiene CAS# 106-99-0
Method	
Method/guideline followed	No data.
Type	Reverse mutation assay (Ames *Salmonella* test).
System of testing	Bacterial.
GLP	No data.
Year	1990.
Species/Strain	Salmonella typhimurium/TA97, TA98, TA100, TA1535.
Metabolic activation	With and without.
Species and cell type	Rat, mouse, and human liver S9 fraction.
Quantity	0.8 and 4.0 mg protein/plate.
Induced or not induced	Arochlor 1254-induced and uninduced rat, mouse, and human S9.
Concentrations tested	0, 30, 40, 50, and 60% butadiene in air.
Statistical Methods	Not specified.
Remarks for Test Conditions	Concentrations of butadiene gas were metered into specially constructed treatment chambers holding the agar plates overlaid with the bacteria and activation system. Actual gas concentrations were determined by gas chromatography before and after the 48 hour exposure period. Different treatment chambers were used for each activation system and for the non-activated treatment. S9 preparations were made according to the procedure of Ames *et al.* (1975).
Results	1,3-Butadiene (BD) induced revertants only in strain TA1535. Mouse S9 showed slightly higher activity than the uninduced rat or human S9 at 30% 1,3-butadiene in air. At concentrations greater than 30%, the number of revertants decreased in the presence of rat or human S9. Results from the human S9-activated treatments did not differ substantially from those of the non-activated treatments. Arochlor 1254-induced rat S9 gave similar results as mouse S9 (uninduced). Since the response was weak, the S9 concentration was increased from 0.8 mg/plate to 4.0 mg/plate. Increasing the concentration of Arochlor 1254-induced rat S9 had no effect on the number of revertants; slightly more revertants were observed using 4.0 than 0.8 mg/plate of uninduced rat S9.
Conclusions	
(study author)	*Salmonella typhimurium* reverse gene mutation (Ames) tests of 1,3-butadiene using strains TA1535, TA97, TA98, and TA100 and employing rat, mouse, and human liver S9 metabolic systems were barely 2-fold above background only in strain TA1535 at 30% butadiene in air with induced and uninduced rat S9 and mouse S9 (uninduced). In general, 1,3-butadiene was a weak *in vitro* genotoxin.
Data Quality	
Reliabilities	Reliable without restrictions. Comparable to guideline study.
Reference	Arce G.T., Vincent D.R., Cunningham M..J, Choy W.N., and Sarrif

	A.M. (1990). *In vitro* and *in vivo* genotoxicity of 1,3-butadiene and metabolites. Environ. Health Perspect. 86:75-8.
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	18-Oct-99

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Butadiene Concentrate, CAS# 68955-28-2. Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
Method	
Method/guideline followed	OECD 482.
Type	Unscheduled DNA Synthesis (UDS).
System of testing	Primary hepatocytes derived from Fischer 344 rats.
GLP	Yes.
Year	1984.
Metabolic activation	No.
Concentrations tested	0, 1000, 5000, 10000, and 20000 ppm.
Control groups and treatment	Negative = air only; positive = 2-acetylaminofluorene (0.2ug/mL).
Statistical Methods	Group means and standard deviations for number of viable cells and nuclear grain counts. The test substance was considered positive if the mean nuclear grain count exceeded the negative control by at least 6 grains per nucleus and the negative control did not exceed 5.
Remarks for Test Conditions	Primary hepatocytes were derived from freshly perfused rat liver (1 male, 10 weeks age, 226 grams body weight). Cultures were seeded with approximately 10^5 cells/mL on Day 1. Three cultures per group were exposed to ^{3}H-thymidine and the test substance for 18-20 hours. The culture flasks were placed in sealed dessicator jars for the exposure period, and the test substance added by injection via a 50cc syringe. Cells growing on coverslips were fixed on Day 2. On Day 3 the slides were dipped in autoradiograph emulsion and stored in the dark at 2-8^{o}C. The autoradiographs were developed and stained on Day 21.
Results	A separate range-finding study was conducted to establish levels of cytotoxicity based on relative cell viability. The test substance was toxic to primary hepatocytes at 10000 ppm where 64% relative viability was observed following 18 hour exposure. At 20000 ppm, the relative viability was 57%. In the UDS study, both positive and negative control groups gave expected responses. A weak positive response was observed at 20000 ppm (7.74 nuclear grain counts vs. 1.24 in the air control vs. 107.13 in the positive control). The 1000, 5000, and 10000 ppm groups were also slightly increased (4.29-5.14) from the air control but less than the criteria for a significant response.
Conclusions (study author)	Cytotoxicity was observed at 10000 ppm. Increased unscheduled DNA synthesis was observed at 20000 ppm.
Data Quality	
Reliabilities	Reliable without restrictions. Guideline study.
Reference	Gulf Oil Chemicals Company (1984). Hepatocyte Primary Culture/DNA Repair Test of Butadiene Feedstock, Unpublished report (Project# 2073).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences,

	Inc.
L*ast changed*	18-Oct-99

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
Method	
Method/guideline followed	Other.
Type	Mammalian cell transformation test.
System of testing	BALB/3T3-A31-1-1 cells.
GLP *Year*	Yes. 1983.
Metabolic activation	No.
Concentrations tested	0, 1000, 5000, 10000, and 20000 ppm.
Control groups and treatment	Negative = air only; positive = 3-methylcholanthrene (1.0 ug/mL).
Statistical Methods	Group means and standard deviations for number of viable cells, cloning efficiency, and transformed foci per culture. The test substance was considered positive if there was a two-fold increase in foci compared to the negative control group.
Remarks for Test Conditions	Each treatment group consisted of 12 flask cultures for cell transformation seeded with 10000 cells and 2 plate cultures for cloning efficiency with 250 cells. The cultures were placed in sealed dessicator jars and exposed to the test substance for two days. The test substance was added to the jars by injection via a 50cc syringe and samples of the exposure atmosphere were analyzed by gas chromatography. The mediums were changed on Day 4 and then weekly. Plate cultures were fixed and stained on Day 8 and flask cultures on Day 29. Foci in transformation cultures were counted and examined microscopically to determine type.
Results	Cloning efficiency was used as a measure of toxicity under culture conditions. Toxicity was observed at 5000 ppm where a relative cloning efficiency of 53.8% was observed. The negative and positive control gave expected responses for transformation. The response for the test substance was not increased from the negative control group at any level tested.
Conclusions	
(study author)	The test substance was negative for cell transformation.
Data Quality	
Reliabilities	Reliable without restrictions. Comparable to draft OECD guideline.
Reference	Gulf Oil Chemicals Company (1983). BALB/3T3 Transformation Test Using Butadiene Feedstock, Unpublished report (Project# 2074).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	18-Oct-99

Genetic Toxicity - *in vitro*

Test Substance	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene.
Method	
Method/guideline followed	No data.
Type	Reverse mutation assay (Ames *Salmonella* test).
System of testing	Bacterial.
GLP Year	Yes. 1985.
Species/Strain	Salmonella typhimurium/ TA98, TA100, TA1535, TA1537, TA1538.
Metabolic activation	With and without.
Species and cell type	Rat liver S9 fraction.
Quantity	0.6 mL.
Induced or not induced	Arochlor 1254-induced.
Concentrations tested	25, 50, 75, or 100 uL.
Statistical Methods	The test substance was considered mutagenic if it produced a dose-related two-fold increase in mean revertant value compared to the negative control.
Remarks for Test Conditions	The test substance was stored in a dry ice/ethanol slurry to prevent loss of volatile components and dosed by microdispenser into sterile septa-capped culture tubes. Sodium phophate buffer or S-9/bacteria mix was injected through the septa into the tubes containing the test substance and pre-incubated for 20 minutes at 37°C. After the pre-incubation period, the contents of the tubes were overlayed on agar and incubated for 48 hours at 37°C. Revertant colonies were counted by automatic colony counter. Positive control chemicals were: 2.0 ug 2-aminoanthracene, 15.0 ug 9-aminoacridine, 20.0 ug 2-nitrofluorene, and 5.0 ug N-methyl-N-nitro-N-nitrosoguanidine, in 50 µl DMSO per plate.
Results	A preliminary toxicity/initial mutagenicity assay was conducted over a range of 10 to 500 µl per plate in two strains (TA100 and TA1537) with and without S-9. Toxicity was exhibited at ≥75uL in TA100, and ≥100uL in TA1537. Some inconsistencies in toxicity with increasing dose level were noted that were attributed to the volatility of the test substance. Based on the toxicity data, the test substance was tested in the pre-incubation mutagenicity assay at volumes of 25, 50, 75, and 100 µl per plate. None of the five strains with or without induced rat liver S-9 exhibited reversion frequencies substantially different from spontaneous controls in this assay.
Conclusions	
(study author)	The test substance was not considered a mutagen with or without metabolic activation in this test system.
Data Quality	

Reliabilities	Reliable without restrictions. Comparable to guideline study.
Reference	Mobil Environmental and Health Sciences Laboratory (1985). An Ames Salmonella/Mammalian Microsome Mutagenesis Assay For Determination of Potential Mutagenicity of Butadiene Concentrate, Unpublished report (Study No. 41653).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	24-Oct-99

Genetic Toxicity - *in vitro*

Test Substance	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 67% 1,3-butadiene, 30% butenes, 2% 1,2-butadiene.
Method	
Method/guideline followed	Other.
Type	Mouse lymphoma mutagenesis assay.
System of testing	Mammalian cell.
GLP Year	Yes. 1985.
Species/Strain	Mouse lymphoma cells/ L5178Y (TK+/-; subclone 3.7.2C).
Metabolic activation	With and without.
Species and cell type	Rat liver S9 fraction.
Quantity	4.0 mL.
Induced or not induced	Arochlor 1242/1254-induced.
Concentrations tested	Nonactivated assays: 10.0, 12.5, 15.0, 17.5, 20.0, 22.5, 25.0, 27.5, 30.0, 35.0 40.0, or 45.0 uL/mL media. S-9 activated assays: 2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5, 20. 0, 22.5, or 25.0 uL/mL.
Statistical Methods	The test substance was considered mutagenic if it produced a dose-related or toxicity-related two-fold increase in average mutant frequency compared to the negative controls, at concentrations exhibiting accepta ble total growths (10% or greater).
Remarks for Test Conditions	The positive control chemical for the S-9 activated assays was 7, 12-dimethylbenz[a]anthracene (DMBA) at 2.5 and 5.0 ug/mL, and ethylmethane sulfonate (EMS) for the nonactivated assays at 0.5 and 1.0 uL/mL. An initial toxicity assay was performed with and without activation at concentrations ranging from 10 to 100 uL/mL. The dosing regimen for the mutagenesis assay was designed to produce 10-90% lethality. Six mLs of cell suspension (10^6 cells/mL) were exposed for 3 hours to the test or positive control substances. An expression period of 2 days followed with determinations of cell population densities and growth. Cultures selected for mutant analysis and cloning efficiencies were incubated for 10-12 days.
Results	Without activation, mutant frequencies and total number of mutants were significantly increased at the two highest concentrations (20.0 and 22.5 uL/mL). Although total growth was very low (5.1% and 5.5%), these levels were considered mutagenic since there was no reduction in cloning efficiency. There were no significant differences in mutant frequency for the S-9 activated cultures.
Conclusions	
(study author)	The test substance induced a significant increase in mutant frequency of mouse lymphoma cells without metabolic activation, but was evaluated as non-mutagenic in the presence of S-9 activation.
Data Quality	

Reliabilities	Reliable without restrictions. Comparable to guideline study.
Reference	Mobil Environmental and Health Sciences Laboratory (1985). Evaluation of the Mutagenic Potential of Butadiene Concentrate in the Mouse Lyphoma (L5178Y/TK+/-) Mutagenesis Assay, Unpublished report (Study No. 41654).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	24-Oct-99

Genetic Toxicity - *in vivo*

Test Substance	
Remarks	1,3-butadiene CAS# 106-99-0
Method	
Method/guideline followed Type	Other. Mammalian erythrocyte micronucleus assay.
GLP	No data.
Year	1994.
Species	Rat and mouse.
Strain	Rat: Wistar. Mouse: CB6F1
Sex	Rat: Male. Mouse: Female.
Route of administration	Inhalation (gas).
Doses/concentration levels	0, 50, 200, or 500 ppm.
Exposure period	6 hours/day for 5 days.
Statistical methods	Student's two-tailed t-test for differences between groups.
Remarks for Test Conditions.	Twenty female CB6F1 mice (approximately 25g, 8-10 weeks old) and ten male Wistar rats (300-350g, 10 weeks old) per group were exposed for 5 days, 6 h/day 0, 50, 200, or 500 ppm of 1,3-butadiene (BD) by inhalation. An additional high concentration group of mice was exposed to 1300 ppm. Exposure concentrations were monitored by infrared spectroscopy (rats) and gas chromatography (mice). The animals were sacrificed 1 day after the last exposure and smears of blood and bone marrow erythrocytes were prepared and stained.
Results	In the rats, no effects on micronuclei frequencies were observed either in the peripheral blood or bone marrow at all exposure levels. A slight toxic effect in rat bone marrow cells (decreased polychromatic/normochromatic ratio) was observed at the 500 ppm level. In the mice, a clear dose-dependent increase in micronuclei frequency was observed in both blood and bone marrow cells at all exposure levels tested.
Conclusions	
(study author)	1,3-butadiene was active in inducing micronuclei in peripheral blood and bone marrow erythrocytes in mice at levels $\geq$50 ppm, but not in rats. The genotoxic effects observed in this study parallel the species differences observed in cancer studies.
Data Quality	
Reliabilities	Reliable without restrictions. Comparable to guideline study.
References	Autio, K., Renzi, L., Catalan, J., Albrecht, O.E., and Sorsa, M. (1994). Induction of Micronuclei in Peripheral Blood and Bone Marrow Erythrocytes of Rats and Mice Exposed to 1,3-Butadiene by Inhalation. Mut. Res. 309:315-320.
	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	25-Oct-99

Genetic Toxicity - i*n vivo*

Test Substance	
Remarks	Butadiene Concentrate, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
Method	
Method/guideline followed	OECD 474
Type	Mammalian erythrocyte micronucleus test
GLP	Yes
Year	1984
Species	Mouse
Strain	Crl:CD-1 BR Swiss
Sex	Male and female
Route of administration	Inhalation (gas)
Doses/concentration levels	10,780; 20,671; 35,430 ppm
Exposure period	2 hours/day for 2 consecutive days
No. of animals per dose	10/sex/group
Control groups and treatment	10/sex negative (air) control; 5/sex positive control (cyclophosphamide, 75 mg/kg intraperitoneal injection)
Statistical methods	Group mean body weights, total polychromatic erythrocytes (PCEs), normochromatic erythrocytes (NORMs), PCEs with micronuclei, and NORMs with micronuclei were compared by t-test ($p<0.05$ = positive).
Remarks for Test Conditions.	Mice were 11 weeks old and 25-42 grams weight at study initiation. Test and control substances were administered on Days 1 and 2. Exposure concentrations determined by gas chromatography. Animals were observed daily and body weights were recorded on Days 1, 3, and 4. Five mice/sex/group were sacrificed on Days 3 and 4 and bone marrow smears prepared; positive controls (5/sex) were sacrificed on Day 3 only.
Results	No mice died during the study; the only clinical observations were an apparent unconsciousness during exposure. There were no significant body weight differences. The negative and positive control groups produced negative and positive resulats, respectively. Mice in the exposed groups showed increased micronuclei formation at all levels in both sexes. Females were statistically increased from control at all levels on Day 3 and at 20,671 ppm and 35,430 ppm on Day 4; males were significantly increased only at 35,430 ppm on both days. There was no significant change in the PCE/NORM ratio in any group.
Conclusions	
(study author)	The test material produced an increased frequency of micronucleated erythrocytes in the bone marrow of mice at all levels tested.
Data Quality	
Reliabilities	Reliable without restrictions. Guideline study.
References	Gulf Oil Chemicals Company (1984). Micronucleus Test in Mouse Bone Marrow: Butadiene Feedstock Administered by

	Inhalation For 2 Hours/Day For 2 Days, Unpublished report (Project #2014).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	13-Oct-99

Repeated Dose Toxicity

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Rubber grade, containing 0.02% t-butyl catechol; purity ≥98.94%.
Method	
Method/guideline followed	Other
Test type	14-week inhalation study
GLP	Yes
Year	1977
Species	Mouse
Strain	B6C3F1
Route of administration	Inhalation (gas)
Duration of test	14 weeks
Doses/concentration levels	0, 625, 1250, 2500, 5000, or 8000 ppm
Sex Exposure period	10 male, 10 female per group 6 hours/day
Frequency of treatment	5 days/week, total of 63 or 64 exposures
Control group and treatment	10 male, 10 female, air-only exposed
Post exposure observation period	Not applicable
Statistical methods	Group means and standard deviations calculated for body weights.
Test Conditions	Groups of 10 mice/sex /group (4-5 weeks age at study initiation) were exposed to various levels of 1,3-butadiene for 6 hrs/day, 5 days/week for 14 weeks (64 exposures). Because four male mice in the high exposure group died by day 4, another 2 groups of 10 male mice each were restarted (control and 8000 ppm). Mice were observed once daily for morbidity and mortality; moribund animals were sacrificed. Body weights were recorded weekly. At the end of the 95 or 93-day (restart) studies, surviving mice were sacrificed. Necropsies were performed and tissues preserved. Histopathologic examinations were performed on all controls, high exposure (8000 ppm), and early deaths.
Results	
NOAEL (NOEL)	1250 ppm.
LOAEL (LOEL)	2500 ppm, based on reduced body weight gains.
Remarks	Six of ten males and 1/10 females exposed at 8000 ppm, 6/10 males and 1/10 females at 5000 ppm, and 1/10 males at 2500 or 1250 ppm died prior to study termination or were sacrificed in a moribund condition. Body weight gains were decreased in males at 2500, 5000, and 8000 ppm, and at 5000 and 8000 ppm in the females. No exposure-related histopathologic effects were observed in the high (8000 ppm) group.
Conclusions	Based on the results of this study, exposure levels of 625 and 1250 ppm were selected for a 2-year carcinogenicity study in

	mice based on reduced body weight gains and mortality in higher exposure groups.
Data Quality	
Reliabilities	Reliable with restrictions. Acceptable, well-documented study report but deficient by current guidelines. No organ weights, hematology or clinical chemistry evaluations were performed.
References	National Toxicology Program, Toxicology and Carcinogenesis Studies of 1,3-Butadiene (CAS No. 106-99-0) in B6C3F1 Mice (Inhalation Studies), NTP Technical Report Series No. 288, NIH Publication 84-2544 (1984).
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	8-Dec-99

Repeated Dose Toxicity

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity >99.2%, containing 120 ppm t-butyl catechol.
Method	
Method/guideline followed	Other.
Test type	13-week inhalation study.
GLP	No data.
Year	1977.
Species	Rat.
Strain	CD (Sprague-Dawley).
Route of administration	Inhalation (gas).
Duration of test	14 weeks.
Doses/concentration levels	0, 1000, 2000, 4000, or 8000 ppm.
Sex	40 male, 40 female per group.
Exposure period	6 hours/day.
Frequency of treatment	5 days/week for 13 weeks.
Control group and treatment	40 male, 40 female, exposed to filtered air only.
Post exposure observation period	Not applicable.
Statistical methods	Analysis of variance for body weights, food consumption, urinalysis, hematology, clinical chemistry, organ weights.
Test Conditions	Groups of 40 rats/sex /group (approx. 5 weeks age at study initiation) were exposed to various levels of 1,3-butadiene for 6 hrs/day, 5 days/week for 13 weeks. All animals were observed daily; individual body weights and food consumption were recorded weekly. Interim sacrifices of 10 rats/sex/group were performed after 2 and 6 weeks of exposure. Three urine samples were obtained from each animal during the 1-2 weeks prior to sacrifice. Blood samples were collected from all rats prior to the 2, 6, and 13 week sacrifices. Brain cholinesterase activity was measured using half the brain of 5 rats/sex/group at the 2 and 6-week sacrifices and all rats at the terminal sacrifice. Organ weights were recorded for the adrenals, brain, gonads, heart, kidneys, liver, lung, pituitary, spleen, and thyroid. Necropsies were performed and tissues preserved. Histopathologic examinations were performed on all control and high exposure (8000 ppm) tissues.
Results	
NOAEL (NOEL)	8000 ppm.
LOAEL (LOEL)	>8000 ppm.
Remarks	Increased salivation was observed in the females after 8 weeks exposure and decreased grooming (stained fur) in the males after 10 weeks. No other exposure-related conditions were observed. Male rats showed slight (non-statistically significant) reductions in body weight gains compared to the controls; female body weights at 1000 and 4000 ppm were statistically higher than the controls.

	Neuromuscular function tests using a modified rotating cone gave some random group differences, but were not considered exposure-related. There were no toxicologically significant differences in hematology, blood chemistry, brain cholinesterase measurements, or urine analysis. Organ weight and organ to brain weight ratios showed some scattered statistically significant differences among the groups but did not indicate any treatment-related effects. Microscopic examination of the tissues of the exposed rats showed a similar incidence and severity of histopathologic findings to the control group.
Conclusions	
(study author)	Rats exposed to butadiene gas at concentrations up to 8000 ppm showed no significant effects related to exposure.
Data Quality	
Reliabilities	Reliable without restrictions. Comparable to guideline study.
References	Crouch, C.N., Pullinger, D.H., and Gaunt, I.F. (1979) Inhalation Toxicity Studies With 1,3-butadiene - 2. 3 Month Toxicity Study in Rats. Am. Ind. Hyg. Assoc. J. 40:796-802.
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	18-Oct-99

Repeated Dose Toxicity

Test Substance	
Remarks	Butadiene feedstock, CAS# 68955-28-2 Gases (petroleum) light steam-cracked, butadiene conc. Approximately 45% 1,3-butadiene, 20% butanes, and 30% butenes.
Method	
Method/guideline followed	Other.
Test type	9-day inhalation study.
GLP	Yes
Year	1982
Species	Rat
Strain	Fischer 344
Route of administration	Inhalation (gas)
Duration of test	12 days (9 exposures)
Doses/concentration levels	0, 2500, and 25100 mg/m3 (0, 1110, and 11140 ppm)
Sex	5 male, 5 female per group.
Exposure period	6 hours/day.
Frequency of treatment	9 exposure days
Control group and treatment	5 male, 5 female, exposed to air only.
Post exposure observation period	Not applicable.
Statistical methods	Bartlett's test and analysis of variance for body and organ weights. If the Bartlett's test indicated homogeneity, Dunnett's test was also performed; if non-homogeneous, a modified t-test was done.
Remarks for Test Conditions	Three groups of 5 rats/sex /group (8 weeks age and 120-198 grams at study initiation) were exposed to 0, 2500, or 25100 mg/m3 of the test substance for 6 hrs/day for a total of 9 exposures. The exposure regimen was 5 days of exposure , 2 days off, 4 days of exposure, then one day for the terminal sacrifice (12 days). Analytical chamber concentrations were determined by gas chromatography, 5 to 16 times per day in the low and high exposure chambers or approximately every 1.5 hours for the control chamber. A particle size sample was performed once daily for each exposure chamber to confirm the absence of aerosol. Individual animal observations were performed twice daily on exposure days and once daily on non-exposure days. Body weights were recorded prior to the first exposure and on Days 1, 7, and 12. Blood samples were obtained from all rats prior to sacrifice on Day 12. A gross necropsy was performed and organ weights recorded for the brain, heart, kidneys, liver, lung, and spleen. These organs plus the testes and ovaries were preserved and examined microscopically.
Results	
NOAEL (NOEL) LOAEL (LOEL)	11140 ppm >11140 ppm
Remarks	Most rats in both exposure groups appeared normal throughout

Conclusions	the study. Nasal discharge was observed in some rats of both groups, and at a greater incidence in the high exposure group. There were no statistically significant differences between the control and exposed groups for mean body weight, organ weight, hematology, or blood chemistry values. There were no exposure-related histopathologic changes in any of the organs and tissues examined.
(study author)	The 9-day repeated inhalation exposure of up to 11140 ppm (25100 mg/m3) resulted in no significant adverse effects in rats.
Data Quality	
Reliabilities	Reliable without restrictions. Comparable to guideline study (OECD 412).
References	Gulf Oil Chemicals Company (1983). Nine-day Repeated Dose Inhalation Study in Rats Using Butadiene Feedstock, Unpublished report (Project #82-090). (1983). Gulf Life Sciences Center, Pittsburgh PA
Other	Robust summary prepared by ExxonMobil Biomedical Sciences, Inc.
Last changed	19-Oct-99

Developmental Toxicity/Teratogenicity

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
Method	
Method/guideline followed	OECD 414.
Test type	Developmental toxicity (teratogenicity) study.
GLP	Yes.
Year	1987.
Species	Mouse.
Strain	CD-1 (Swiss).
Route of administration	Inhalation (gas).
Concentration levels	0, 40, 200, or 1000 ppm.
Sex	18-22 pregnant females per group.
Exposure period	Days 6-15 of gestation.
Frequency of treatment	6 hours/day.
Control group and treatment	Air-exposed only.
Duration of test	Females sacrificed on gestation day 18.
Statistical methods	Analysis of variance for body weights, number of resorptions, implants, live, dead or affected fetuses per litter. Significant differences among the groups were also analyzed by Duncan's multiple range test or arcsin transformation of the response proportion. Binary-response variables were between groups were compared using chi-square or Fisher's exact test.
Remarks for Test Conditions.	Female mice were mated to unexposed males and exposed from days 6-15 of gestation to 0, 40, 200, or 1000 ppm of the test substance. Analytical chamber concentrations were measured by on-line gas chromatography. Body weights were recorded on gestation days 0, 6, 11, 16, and 18. Maternal animals were observed daily for mortality, morbidity, and signs of toxicity and examined for gross tissue abnormalities at necropsy (day 18). The uterus and placenta was removed and weighed; the number of implantation sites, resorptions, live and dead fetuses were recorded. Live fetuses were weighed and subjected to external, visceral, and skeletal examinations. Approximately 50% of the fetal heads were sectioned and examined.
Results	
NOAEL maternal toxicity	40 ppm.
NOAEL developmental	40 ppm.
toxicity	There were decreases in maternal body weight gains in the 200 and 1000 ppm groups. Fetal weights were significantly reduced in both males and females at 200 and 1000 ppm; placenta weights were significantly reduced for corresponding male fetuses at 200 ppm and for both males and females at 1000 ppm. There were no significant differences in percent resorptions or malformations per litter, although there was an increase in fetal variations (supernumary ribs and reduced ossification of sternebrae) at 200 and 1000 ppm.
Conclusions	

(study author)	Developmental toxicity was observed in mice in the presence of maternal toxicity at 200 and 1000 ppm. A slight statistically significant decrease in male fetal weight (95% of control) was also observed, but the biological significance of this finding has been questioned.
Data Quality	
Reliabilities	Reliable without restrictions. Guideline study.
References	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
La*st changed*	20-Oct-99

Developmental Toxicity/Teratogenicity

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
Method	
Method/guideline followed	OECD 414.
Test type	Developmental toxicity (teratogenicity) study.
GLP	Yes.
Year	1987.
Species	Rat.
Strain	CD (Sprague-Dawley).
Route of administration	Inhalation (gas).
Concentration levels	0, 40, 200, or 1000 ppm.
Sex	24-28 pregnant females per group.
Exposure period	Days 6-15 of gestation.
Frequency of treatment	6 hours/day.
Control group and treatment	Air-exposed only.
Duration of test	Females sacrificed on gestation day 20.
Statistical methods	Analysis of variance for body weights, number of resorptions, implants, live, dead or affected fetuses per litter. Significant differences among the groups were also analyzed by Duncan's multiple range test or arcsin transformation of the response proportion. Binary-response variables between groups were compared using chi-square or Fisher's exact test.
Remarks for Test Conditions.	Female rats were mated to unexposed males and exposed from days 6-15 of gestation to 0, 40, 200, or 1000 ppm of the test substance. Analytical chamber concentrations were measured by on-line gas chromatography. Body weights were recorded on gestation days 0, 6, 11, 16, and 20. Maternal animals were observed daily for mortality, morbidity, and signs of toxicity and examined for gross tissue abnormalities at necropsy (day 20). The uterus and placenta was removed and weighed; the number of implantation sites, resorptions, live and dead fetuses were recorded. Live fetuses were weighed and subjected to external, visceral, and skeletal examinations. Approximately 50% of the fetal heads were sectioned and examined.
Results	
NOAEL maternal toxicity	200 ppm
NOAEL developmental	1000 ppm
toxicity	The only toxicity observed was decreased body weight gains in the dams at 1000 ppm. The percentage of pregnant animals and number of litters with live fetuses were unaffected by treatment. There were no significant differences among the groups for number of live fetuses per litter, percent resorptions or malformations per litter, placental or fetal body weights, or sex ratio.
Conclusions	

(study author)	There was no evidence of teratagenicity or adverse reproductive effects in any of the exposed groups.
Data Quality	
Reliabilities	Reliable without restrictions. Guideline study.
References	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
Other	Robust Summary Prepared by ExxonMobil Biomedical Sciences, Inc.
La*st changed*	20-Oct-99

Toxicity to Re production

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
Method	
Method/guideline followed	Other.
Test type	Sperm-head morphology assay.
GLP	Yes.
Year	1987.
Species	Mouse.
Strain	B6C3F1.
Route of administration	Inhalation (gas).
Concentration levels	0, 200, 1000, and 5000 ppm.
Sex	20 males per group.
Exposure period	6 hours/day.
Frequency of treatment	5 days.
Control group and treatment	Air-exposed only.
Duration of test	Males sacrificed 5 weeks post-exposure.
Statistical methods	Normal and abnormal sperm heads were expressed as percentage of the total number of cells examined. These data were subjected to arcsin transformation and evaluated by analysis of variance. If significant, Duncan's multiple range test was used for intergroup differences. Dose response trends were determined by orthogonal contrast.
Remarks for Test Conditions.	The mice were observed twice daily and body weights recorded weekly. During the fifth week post-exposure the mice were sacrificed and examined for lesions of the reproductive tract and other gross abnormalities. Sperm was obtained from the cauda of the right epididymis. Slides were prepared, stained, and examined microscopically. The morphology of at least 500 sperm heads per mouse was categorized.
Results	
NOAEL	200 ppm The percentage of abnormal sperm heads increased with exposure concentration: 1.61% (0 ppm), 1.95% (200 ppm), 2.79% (1000 ppm), and 3.79% (5000 ppm). Only the values for the 1000 and 5000 ppm groups were significantly different from the control ($p < 0.05$). Only a single timepoint was examined, so the effect on all stages of spermatogenesis could not be determined.
Conclusions	
(Study author)	These results suggest that the test substance affected spermatogenesis in mice at 1000 and 5000 ppm, but the effect of this observation on other reproductive endpoints is not known.
Data Quality	
Reliabilities	Reliable with restrictions. Acceptable, well-documented publication which meets basic scientific principles.
References	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R.,

	Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
Other	Robust Summaries Prepared by ExxonMobil Biomedical Sciences, Inc.
La*st changed*	20-Oct-99

Toxicity to Reproduction

Test Substance	
Remarks	1,3-butadiene, CAS# 106-99-0 Purity 99.88%
Method	
Method/guideline followed	Other.
Test type	Rodent dominant lethal test.
GLP	Yes.
Year	1987.
Species	Mouse
Strain	CD-1 (Swiss).
Route of administration	Inhalation (gas).
Concentration levels	0, 200, 1000, and 5000 ppm.
Sex	20 males per group.
Exposure period Frequency of treatment	6 hours/day. 5 days.
Control group and treatment	Air-exposed only.
Duration of test	8 weeks post-exposure.
Statistical methods	The number of implantation sites and intrauterine deaths per litter for each week were analyzed by analysis of variance. When appropriate, proportions of resorptions and dead or live fetuses per implant were subjected to arcsin transformation and evaluated by analysis of variance. If significant, Duncan's multiple range test was used for intergroup differences.
Remarks for Test Conditions.	After five days of exposure, the male mice were mated with unexposed females (two females per week for each male for 8 consecutive weeks). Females were removed from cohabitation after 7 days sacrificed 12 days later and the uterine contents examined. Observations included: the total number, position, and status of implantations; the numbers of early and late resorptions; and numbers of live and dead fetuses.
Results	Slight statistically significant effects were noted in the mated females for three endpoints during the first 2 weeks post-exposure: ratio of dead to total implants, percentage of females with $\geq$2 dead implants, and number of dead implants per pregnancy. However, these observations only occurred in the two lower exposure groups (except for increased number dead implants/pregnancy in the 5000 ppm group during week 1). There were no differences for number of pregnant females, implantations per litter, number of live fetuses, dead implantations per total implantations, or number of resorptions during weeks 1 and 2. There were no differences for any endpoint during weeks 3-8.
Conclusions	
(Study author)	The authors concluded that the results observed during the first two weeks are consistent with an adverse effect on more mature germ cells (spermatozoa and spermatids) however considering the lack of effects in the high exposure group the findings are not clear for a

	dose-dependent response.
Data Quality	
Reliabilities	Reliable with restrictions. Acceptable, well-documented publication which meets basic scientific principles.
References	Morrissey, R.E., Schwetz, B.A., Hackett, P.L., Sikov, M.R., Hardin, B.D., McClanahan, B.J., Decker, J.R., and Mast, T.J. (1990). Overview of Reproductive and Developmental Toxicity Studies of 1,3-Butadiene in Rodents. Environ. Health Perspect. 86:79-84.
Other	Robust Summary Prepared by Exxon Biomedical Sciences, Inc.
Last *changed*	20-Oct-99

Genetic Toxicity - *in vivo*

Test Substance	
Remarks	C4 Crude Butadiene (Low 1,3-Butadiene Content) approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS #: 68476-52-8 Other CAS #s in the stream: 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7.
Method	
Method/guideline followed Type	U.S. EPA OPPTS 870.5395 (1998) and OECD # 474 (1997) guidelines. Mammalian erythrocyte micronucleus assay.
GLP	Yes.
Year	2001.
Species	Mouse.
Strain Sex	B6C3F1 Male and Female
Route of administration	Inhalation (gas).
Doses/concentration levels	0, 0.5, 10.0, or 20.0 mg/L.
Exposure period	4 hours/day for 2 days.
Statistical methods	The raw data on the counts of MN-PCE for each animal were first transformed by adding one (1) to each count and then taking the natural log of the adjusted number. The transformed MN-PCE data and the data on percent PCE were analyzed separately by a two-way analysis of variance (Winer, 1971). The sex-by-dose interaction in the two-way analysis was reviewed and if significant, a one-way analysis was performed for each sex. Pairwise comparisons of treated vs. control groups were done, if the dose effect was significant, by Dunnett's t-test, one-sided (upper) for MNPCE and two-sided for the percent PCE (Winer 1971). Linear dose-related trend tests were performed only if any of the pairwise comparisons yielded significant differences. The alpha level at which all tests were conducted was 0.05.
Remarks for Test Conditions.	Groups of six male B6C3F1 mice (approximately 26g, 9 weeks old) and six female B6C3F1 mice (approximately 21g, 9 weeks old) were exposed whole-body inhalation to target concentrations of 0, 0.5, 10.0, and 20.0 mg/L of the C4 Crude Butadiene, Low 1,3-Butadiene Content. All inhalation exposures occurred under dynamic airflow conditions and chamber concentrations were monitored by analytical methods. Inhalation exposures occurred on two consecutive days, 4 hours per day. A positive control group was dosed by oral gavage with 120 mg/kg of cyclophosphamide approximately 24 hours before sacrifice. Groups of animals (6/sex/dose) were sacrificed at 24 hours after the second treatment for the collection of femoral bone marrow to evaluate the incidence of micronuclei (MN) in polychromatic erythrocytes (2000 PCE/animal) The proportion of PCE among erythrocytes in the bone marrow was estimated by examining 200

	erythrocytes/animal.
Results	Statistically significant increases in the frequencies of MN-PCE in both sexes of all groups treated with the test material were observed as compared to the negative controls. Although statistical analyses indicated a significant dose response, the difference in MN-PCE incidence at the high- (20 mg/L) and low- (0.5 mg/L) dose was minimal. The positive control treatment induced a significant increase in the frequency of MN-PCE. The mean proportion of PCE among the erythrocytes (200/animal) in the bone marrow was not affected following exposure to the test material while the positive control treatment significantly reduced this value.
Conclusions	
(study author)	C4 Crude Butadiene (low 1,3-butadiene content) was positive for the induction of micronuclei in this test system under the experimental conditions used.
Data Quality	
Reliabilities	Reliable without restrictions.
References	Organisation for Economic Co-Operation and Development (OECD) (1997). Guidelines for Testing of Chemicals. #474. Genetic Toxicology: Micronucleus Test, OECD Publication Service, 2 Rue Andre-Pascal, 75775 Paris Cedex 16, France. U.S. EPA (1998). Office of Prevention, Pesticides and Toxic Substances, OPPTS 870.5395. *In Vivo Mammalian Bone Marrow Cytogenetic Tests - Micronucleus assay* Winer, B. J. (1971). *Statistical Principles in Experimental Design* (2nd Edition). McGraw-Hill, New York, New York. Spencer, T.J., Hammond, T.A., Houtman, C.E. and Marty, G.T. (2001). The valuation of C4 crude butadiene (low 1,3-butadiene content) in the mouse bone marrow micronucleus test by an inhalation exposure - multiple exposures followed by a single sampling point. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.
Other	Last updated: Robust summary prepared by contractor to Olefins Panel

Repeated Dose Toxicity

Test Substance	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content), approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream : 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes
Year	2001
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	36-37 days
Doses/concentration levels	0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3)
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights, body weight gains, feed consumption, organ weights, clinical chemistry data and appropriate hematologic data were evaluated by ANOVA. Detailed clinical observation incidence scores for ranked observations and sensory evaluation scores were statistically analyzed by a z-test of proportions. Rectal temperature and grip performance were analyzed by an analysis of covariance with dose as the factor and time as the covariate. Motor activity was analyzed by a repeated-measure design with treatment as a between-subjects factor and the repeated factor of time.
Test Conditions	Groups of 12 male and 12 female CD rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3). The main study (repeated-exposure general toxicity and neurotoxicity endpoints) males and females were exposed for 36 and 37 days, respectively. Effects on general toxicity, neurobehavioral activity, clinical chemistry, and hematology were evaluated. In addition, a gross necropsy with extensive histopathologic examination of tissues was conducted. The study also contained reproductive and developmental toxicity satellite groups (summarized separately).

Results	
NOAEL (NOEL)	20 mg/L (20,000 mg/mg^3).
LOAEL (LOEL)	Not applicable.
Remarks	Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L (2,000; 10,000; or 20,000 mg/m^3) exposure groups were **2.17** ± 0.461, **9.81** ± 1.66, **19.1** ± 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity. There were no deaths or treatment-related clinical observations noted. No significant differences in body weights or feed consumption were observed for the males or females at any dose level tested throughout the duration of the study. Sensory evaluation, rectal temperature, and fore/hindlimb grip performance data revealed no treatment-related findings. Treatment did not affect motor activity total counts (treatment-by-time interaction, p = 0.0930). However, the treatment-by-time-by-epoch interaction was significant (p = 0.0098). Examination of the data suggested that this effect could be reasonably attributed to the significant time-by-epoch interaction (p = 0.0001) rather than to a true treatment effect. This was confirmed following calculation of linear contrasts to determine which group(s), if any, were different from the control group. These analyses revealed that none of the three treatment groups were significantly different from control (alpha > 0.02) when the time-by-epoch-by-treatment interaction was considered. There were no treatment-related changes for males and females at any dose level for prothrombin time, hematology values or clinical chemistry measures. Females exposed to 2 mg/L had a statistically identified increase in hematocrit value, and a statistically identified decrease in serum total protein. Given the lack of dose response, effects on related parameters, and similar effects in males, these were considered incidental findings that were toxicologically insignificant. There were no effects of exposure on organ weights, gross pathology or histopathology in any of the treated groups when compared to their respective controls.
Conclusions	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3) produced no evidence of any adverse effects on clinical observations, organ weights, gross or histopathology, neurobehavioral activity, clinical chemistry or hematology endpoints. Based on these data, the no-observable-effect level

	(NOEL) for repeated dose toxicity was 20 mg/L, the highest concentration tested.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.
Other	
Last changed	6-Aug-01 Robust summary prepared by contract to Olefins Panel

Toxicity to Reproduction

Test Substance	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content) approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream: 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes.
Year	2001
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	Two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until postnatal day 4. The males were exposed for 36-37 days.
Doses/concentration levels	0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3)
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights and feed consumption, maternal body weight gains, and pup body weights were analyzed by ANOVA. Gestation length, average time to mating (precoital interval) and litter size were analyzed using a nonparametric ANOVA. Pregnancy rates and mating, conception, fertility and gestation indices were analyzed by the Fisher exact probability test. Evaluation of the neonatal sex ratio was performed by the binomial distribution test. Post-implantation loss, pup survival indices, and other incidence data among neonates were analyzed using the litter as the experimental unit by a censored Wilcoxon test.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3). The study design included a main study for repeated dose toxicity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were

	exposed for two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. Males from the main study were used to breed these females. The dams were allowed to deliver their litters, which were retained until postnatal day 4. Effects on general toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 5. Litter size, pup survival, sex, body weight, and the presence of gross external malformations was assessed in the offspring. The males were exposed for a total of 36 to 37 days, and were then necropsied. In addition to the repeated dose toxicity end points assessed (discussed separately), reproductive assessment of the males included mating, conception and fertility indices, reproductive organ weights and gross/histopathology of the reproductive tract. Testis histopathology included a qualitative assessment of stages of the spermatogenic cycle.
Results	
NOAEL (NOEL)	20 mg/L (20,000 mg/mg^3).
LOAEL (LOEL)	Not applicable.
Remarks	Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L (2,000; 10,000; or 20,000 mg/m^3) exposure groups were **2.17** $\pm$ 0.461, **9.81** $\pm$ 1.66, **19.1** $\pm$ 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity. There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption were observed at any dose level tested throughout the duration of the study. The only exception to this was a statistically identified increase in feed consumption noted for the 10 mg/L satellite females during the premating period (days 7-14). However, this increase was considered spurious, as feed consumption increases were not noted during subsequent gestation and lactation periods and similar changes in feed consumption were not observed at the highest exposure level of 20 mg/L. There were no treatment-related effects at any dose level on any of the reproductive parameters evaluated in this study. These included measures of reproductive performance (mating, conception and fertility, time to mating, gestation length, litter size), offspring survival (gestation and postnatal survival indices, percent pre- and post-implantation loss), pup body weight and pup sex ratio. The only statistically identified

	change in any of these parameters was an increase in post-implantation loss occurring only at the low-dose. This was considered a spurious finding, given the lack of a dose response. Of the 12 females mated in each group, the number of viable litters produced was 11, 11, 11, and 12 for the 0, 2, 10 and 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3) exposure level groups, respectively. External morphological alterations observed in the pups were limited to a hernia observed in a single pup from the high dose group. Given the low incidence of this finding, it was considered spurious and unrelated to exposure.
Conclusions	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L (0; 2,000; 10,000; or 20,000 mg/m^3) produced no evidence of adverse effects on any measures of reproductive function. Based on these data, the no-observable-effect level (NOEL) for reproductive toxicity was 20 mg/L, the highest concentration tested.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council, Olefins Panel.
Other	
Last changed	6-Aug-01 Robust summary prepared by contractor to Olefins Panel

Developmental Toxicity/Teratogenicity

Test Substance	
Remarks	C4 Crude Butadiene (low 1,3-Butadiene Content), approx. composition: 10% 1,3-butadiene, 4% isobutane, 4% n-butane, 29% trans-2-butene, 29% 1-butene, 11% isobutylene, 12% cis-2-butene Primary CAS#: 68476-52-8; Other CAS #s used to represent this stream : 25167-67-3, 64742-83-2, 68187-60-0, 68476-44-8, 68955-28-2, and 68956-54-7
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure inhalation toxicity study with the reproduction / developmental screening test
GLP	Yes.
Year	2001
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (vapor).
Duration of test	Two weeks prior to breeding, during breeding (up to two weeks), and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until postnatal day 4.
Doses/concentration levels	0, 2, 10, or 20 mg/L
Sex	12 male, 12 female per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 male, 12 female, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Adult body weights and feed consumption, maternal body weight gains, and pup body weights were analyzed by ANOVA. Gestation length, average time to mating (precoital interval) and litter size were analyzed using a nonparametric ANOVA. Pregnancy rates and mating, conception, fertility and gestation indices were analyzed by the Fisher exact probability test. Evaluation of the neonatal sex ratio was performed by the binomial distribution test. Post-implantation loss, pup survival indices, and other incidence data among neonates were analyzed using the litter as the experimental unit by a censored Wilcoxon test.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats were exposed to vapors of the test material daily by inhalation for approximately six hours/day at exposure levels of 0, 2, 10, or 20 mg/L. The study design included a main study for repeated dose toxicity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were exposed for two weeks prior to breeding,

	during breeding (up to two weeks), and continuing until day 19 of gestation. Males from the main study were used to breed these females. The dams were allowed to deliver their litters, which were retained until postnatal day 4. Effects on general toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 5. Litter size, pup survival, sex, body weight, and the presence of gross external malformations was assessed in the offspring.
Results	
NOAEL (NOEL)	20 mg/L.
LOAEL (LOEL)	Not applicable.
Remarks	Actual time-weighted averages for total olefins for the 2, 10 and 20 mg/L exposure groups were **2.17** ± 0.461, **9.81** ± 1.66, **19.1** ± 2.63 mg/L, respectively, over the 37 exposure days in the study. Owing in part to the nature of the test material, there were technical difficulties in generating vapors from the test material, such that targeted exposure concentrations were not met on one entire day and for brief periods on a few other days. However, the affected instances were limited relative to the total duration of the study and were considered to have no significant impact on study integrity. There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption were observed at any dose level tested throughout the duration of the study. There were no treatment-related effects at any dose level on any of the reproductive parameters evaluated in this study. These included measures of reproductive performance (mating, conception and fertility , time to mating, gestation length, litter size), offspring survival (gestation and postnatal survival indices, percent pre- and post-implantation loss), pup body weight and pup sex ratio. The only statistically identified change in any of these parameters was an increase in post-implantation loss occurring only at the low-dose. This was considered a spurious finding, given the lack of a dose response. Of the 12 females mated in each group, the number of viable litters produced was 11, 11, 11, and 12 for the 0, 2, 10 and 20 mg/L exposure level groups, respectively. External morphological alterations observed in the pups were limited to a hernia observed in a single pup from the high dose group. Given the low incidence of this finding, it was considered to be a spontaneous finding unrelated to exposure.
Conclusions	Repeated inhalation exposure of C4 Crude Butadiene, Low 1,3-Butadiene to male and female Sprague Dawley rats at levels of 0, 2, 10, or 20 mg/L produced no evidence of developmental toxicity or teratogenicity, as assessed in the OECD 422 study design. Based on these data, the no-observable-effect level (NOEL) for developmental toxicity was 20 mg/L, the highest

	concentration tested.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Carney, E.W., Liberacki, A.B., Thomas, J., Houtman, C.E. and Marable, B.R. (2001). C4 Crude butadiene, low 1,3-butadiene content: a combined repeated exposure inhalation toxicity study with the reproduction/developmental screening test in Sprague Dawley rats. Report of The Dow Chemical Company conducted for the American Chemistry Council Olefins Panel.
Other	
Last changed	6-Aug-01 Robust summary prepared by contractor to Olefins Panel

AQUATIC TOXICITY ROBUST SUMMARIES

Fish Acute Toxicity

Test Substance*:	Other TS
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species: **Analytical Monitoring:**	Freshwater Fish (calculated toxicity values are not species specific) Not applicable
Exposure Period:	96 hours
Statistical Method: (FT - ME)*	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products. Chemical — Calculated log K_{ow} — Measured* log K_{ow} Isobutane — 2.23 — 2.76 n-butane — 2.31 — 2.89 isobutylene — 2.23 — 2.34 cis-butene-2 — 2.09 — 2.31 trans-butene-2 — 2.09 — 2.33 butene-1 — 2.17 — 2.40 1,3-butadiene — 2.03 — 1.99

	* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the fish acute toxicity range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see Test Substance). Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. 3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated fish acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows: Chemical — Calculated log K_{ow} — Fish Acute 96-hr LC50 (mg/L) Isobutane — 2.23 — 26.19 n-butane — 2.31 — 22.03 isobutylene — 2.23 — 25.28 cis-butene-2 — 2.09 — 34.23 trans-butene-2 — 2.09 — 34.23 butene-1 — 2.17 — 28.79 1,3-butadiene — 2.03 — 37.59

	Chemical / Measured* log K_{ow} / Fish Acute 96-hr LC50 (mg/L) Isobutane 2.76 8.32 n-butane 2.89 6.28 isobutylene 2.34 19.93 cis-butene-2 2.31 21.26 trans-butene-2 2.33 20.36 butene-1 2.40 17.50 1,3-butadiene 1.99 40.98 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated Kow values, products in this category are expected to have a fish 96-hour LC50 range of 22.03 to 37.59 mg/L. Based on the measured Kow values, products in this category are expected to have a fish 96-hour LC50 range of 6.28 to 40.98 mg/L.
Reliability: (FT - RL)	(2) Reliable with restrictions The toxicity values are calculated.
Reference: (FT - RE)	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for " acute toxicity to fish ". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

Daphnid Acute Toxicity

Test Substance*:	Other TS
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type): **GLP:**	Acute Daphnid Toxicity Calculation; LC50 Not applicable
Year (study performed):	Not applicable
Species:	Daphnid (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method: (FT - ME)*	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products. Chemical — Calculated log K_{ow} — Measured* log K_{ow} Isobutane 2.23 2.76 n-butane 2.31 2.89 isobutylene 2.23 2.34 cis-butene-2 2.09 2.31 trans-butene-2 2.09 2.33 butene-1 2.17 2.40 1,3-butadiene 2.03 1.99 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured

values.

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the daphnid acute toxicity range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see Test Substance). Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Results: (FT - RS)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Calculated daphnid acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:

Chemical	Calculated log K_{ow}	Daphnid Acute 48-hr LC50 (mg/L)
Isobutane	2.23	28.51
n-butane	2.31	24.11
isobutylene	2.23	27.53
cis-butene-2	2.09	36.91
trans-butene-2	2.09	36.91
butene-1	2.17	31.21
1,3-butadiene	2.03	40.27

Chemical	Measured* log K_{ow}	Daphnid Acute 48-hr LC50 (mg/L)

	Isobutane 2.76 9.39 n-butane 2.89 7.15 isobutylene 2.34 21.86 cis-butene-2 2.31 23.28 trans-butene-2 2.33 22.32 butene-1 2.40 19.28 1,3-butadiene 1.99 43.88 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 24.11 to 40.27 mg/L. Based on the measured Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 7.15 to 43.88 mg/L.
Reliability: (FT - RL)	(2) Reliable with restrictions The toxicity values are calculated.
Reference: (FT - RE)	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for " acute toxicity to aquatic invertebrates ". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

Alga Toxicity

Test Substance*:	Other TS
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type): **GLP:**	Green Alga Toxicity Calculation; EC50 Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Alga (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method: (FT - ME)*	Not applicable
Test Conditions: (FT - TC) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products. Chemical — Calculated log K_{ow} — Measured* log K_{ow} Isobutane 2.23 2.76 n-butane 2.31 2.89 isobutylene 2.23 2.34 cis-butene-2 2.09 2.31 trans-butene-2 2.09 2.33 butene-1 2.17 2.40 1,3-butadiene 2.03 1.99 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more

	than 13,000 organic compounds with reliably measured values.. Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4. The seven chemicals selected to represent the alga toxicity range of this category are C4 hydrocarbons that are common across the 10 CAS numbers (see Test Substance). Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. 3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Results: (FT - RS) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated alga toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows: Chemical — Calculated log K_{ow} — Alga Toxicity 96-hr EC50 (mg/L) Isobutane — 2.23 — 18.06 n-butane — 2.31 — 15.35 isobutylene — 2.23 — 17.44 cis-butene-2 — 2.09 — 23.19 trans-butene-2 — 2.09 — 23.19 butene-1 — 2.17 — 19.71 1,3-butadiene — 2.03 — 25.27 Measured* — Alga Toxicity

	Chemical / log K_{ow} / 96-hr EC50 (mg/L) Isobutane 2.76 6.13 n-butane 2.89 4.71 isobutylene 2.34 13.94 cis-butene-2 2.31 14.81 trans-butene-2 2.33 14.22 butene-1 2.40 12.33 1,3-butadiene 1.99 27.42 * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.
Test Substance: (FT - TS)	25167-67-3 Butenes 68477-41-8 Distillate (Petroleum), Extractive C3-5 68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate 68476-44-8 Hydrocarbons, >C3 68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates 68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked 68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product 68956-54-7 Hydrocarbons C4, Unsaturated 69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product 64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked
Conclusion: (FT - CL)	Based on the calculated Kow values, products in this category are expected to have an alga 96-hour EC50 range of 15.35 to 25.27 mg/L. Based on the measured Kow values, products in this category are expected to have an alga 96-hour EC50 range of 4.71 to 27.42 mg/L.
Reliability: (FT - RL)	(2) Reliable with restrictions The toxicity values are calculated
Reference: (FT - RE)	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source): (FT - SO)	American Chemistry Council, Olefins Panel

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to aquatic plants". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion